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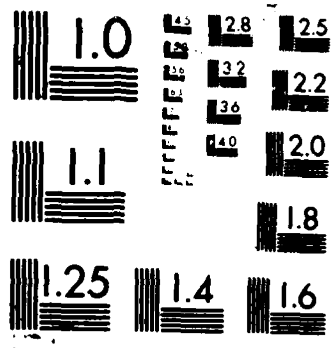
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Lehigh University

THE Ξ FUNCTION

BY

J.D.A. WALKER AND R.K. SCHARNHORST

REPORT FM-9

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This report is a compendium of properties of a mathematical function (the Ξ function) which arises in the modeling of turbulent boundary-layer flows near solid walls. The Ξ function is formally defined as a triple integral which cannot be easily expressed in terms of elementary or known special functions. Thus series and asymptotic expansions are developed here as well as a table of integrals (most of which are indefinity). The function and its derivative are tabulated correct to ten significant figures. A FORTRAN function routine for the calculation of $\Xi(x)$ and $\Xi'(x)$ is also given. Keywords

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THE Ξ FUNCTION

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ABSTRACT

This report is a compendium of properties of a mathematical function (the Ξ function) which arises in the modeling of turbulent boundary-layer flows near solid walls. The Ξ function is formally defined as a triple integral which cannot be easily expressed in terms of elementary or known special functions. Thus series and asymptotic expansions are developed here as well as a table of integrals (most of which are indefinite). The Ξ function and its derivative are tabulated correct to ten significant figures. A FORTRAN function routine for the calculation of $\Xi(x)$ and $\Xi'(x)$ is also given.

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GLOSSARY OF FUNCTIONS AND NOTATION

$E_1(x)$	Exponential integral	$\int_x^\infty \frac{e^{-t}}{t} dt$
$\mathit{erf}(x)$	Error function	$\frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$
$\mathit{erfc}(x)$	Complementary error function	$\frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$
$\mathit{erfei}(x)$	Function discussed in Appendix A	$\int_0^x \frac{\mathit{erf}(t)}{t} dt$
$F(x)$	Dawson's integral	$e^{-x^2} \int_0^x e^{t^2} dt$
G	Catalan's constant	0.91596 55942
$\binom{j}{i}$	Binomial coefficient	$\frac{j!}{(j-i)!i!}$
$(2j+1)!!$	Double factorial	$(2j+1)\cdot(2j-1)\cdot\ldots\cdot5\cdot3\cdot1$
$(2j)!!$	Double factorial	$(2j)\cdot(2j-2)\cdot\ldots\cdot4\cdot2$
γ	Euler's constant	0.57721 56649
$\gamma(a,x)$	Incomplete gamma function	$\int_0^x e^{-t} t^{a-1} dt$
$\Gamma(a)$	Gamma function	$\int_0^\infty e^{-t} t^{a-1} dt$
$\Gamma(a,x)$	Incomplete gamma function	$\int_x^\infty e^{-t} t^{a-1} dt$
$\psi(p)$	Psi function	$\frac{d}{dp} \ln \Gamma(p)$

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1. Introduction

The diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial y^2} , \qquad (1.1)$$

arises in a wide variety of applications in engineering including fluid mechanics and heat and mass transfer. In many situations, the relevant solution of equation (1.1) is a function of the similarity variable,

$$\eta = \frac{y}{2\sqrt{t}} . \qquad (1.2)$$

When the solution of equation (1.1) is required for y (or η) in the semi-infinite range $0 \leq y < \infty$, a boundary condition is normally known at y=0 as well as some particular type of asymptotic behavior as $y \to \infty$. Specific types of asymptotic conditions which can occur might include the following situations:

i) u must approach zero or a constant exponentially, viz.

$$u \sim A_0 \text{ , as } y \to \infty , \qquad (1.3)$$

where A_0 is a constant (or zero);

ii) u must approach zero or a constant algebraically, viz.

$$u \sim A_1 + A_2 f(t)\eta^{-\alpha} \quad \text{as} \quad \eta \to \infty , \qquad (1.4)$$

where f(t) is a function of t, A_1 and A_2 are constants and $\alpha > 0$; and

iii) u must become large algebraically for large y, viz.

$$u \sim A_3 g(t)\eta^{\beta} + \ldots \text{ as } \eta \to \infty , \qquad (1.5)$$

where g(t) is a function of t, A_3 is a constant and $\beta > 0$.

For the types of asymptotic conditions described by equations (1.3), (1.4) and (1.5), the solution to equation (1.1) can often be written in terms of parabolic cylinder functions or alternatively in terms of repeated integrals of the error function (Abramowitz and Stegun, 1964).

A rather different type of asymptotic condition for large y arises in the study of velocity and temperature profiles in the near-wall region of turbulent boundary-layer flows (Black, 1968; Scharnhorst, Walker and Abbott, 1977; Scharnhorst, 1978; Weigand, 1978; Walker, Scharnhorst and Weigand, 1986); here a solution of the diffusion equation is required whose time-average over a finite interval of time is logarithmic for large y. It is in this context that the Ξ function arises.

The details of the turbulence model discussed by Walker, Scharnhorst and Weigand (1986) are complex and will not be discussed here. However an essential feature of the analysis is that a solution of equation (1.1) is required subject to the asymptotic boundary condition,

$$u \sim B \ln y + C \quad \text{as} \quad y \to \infty , \tag{1.6}$$

where B and C are known constants. The solution of equation (1.1) satisfying,

$$u(0,t) = A, \tag{1.7}$$

where A is constant, is given by,

$$u = [C + \frac{B}{2}\{2\ln(2) - \gamma + \ln(t)\}]\ erf(\eta) + A\,erfc(\eta)$$

$$+ \frac{4B}{\sqrt{\pi}}\,\Xi(\eta)\ . \qquad (1.8)$$

Here γ is Euler's constant and the Ξ function is formally defined as the triple integral,

$$\Xi(\eta) = \int_0^{\eta} e^{-\xi^2} \int_0^{\xi} e^{\zeta^2} \int_0^{\zeta} e^{-t^2}\, dt\, d\zeta\, d\xi \ . \qquad (1.9)$$

The function defined by equation (1.9) cannot be easily expressed in terms of elementary or known special functions. Consequently because the function appears in velocity and temperature profile representations of the flow in the near wall region of turbulent boundary layers (Walker, Scharnhorst and Weigand, 1986), it is worthwhile to develop a compendium of useful properties of this function and this is the purpose of this report.

The plan of the report is as follows. In section 2, a number of general properties of the Ξ function are given and $\Xi(x)$ and its derivative $\Xi'(x)$ are plotted in figures 1 and 2 respectively. The notation is generally consistent with Abramowitz and Stegun (1964) and is defined in a separate section on page iv; generally x is used to denote a real variable and a denotes a positive real constant. In section 3, a number of indefinite and definite integrals are listed; for the indefinite integrals, the constants of integration have been omitted. In three of the integrals given in section 3, a new function arises which has been denoted by erfei(x); some properties of this

function are given in Appendix A. Finally a FORTRAN program for the evaluation of Ξ and Ξ' is given in Appendix B as well as tabulated values of these functions correct to ten significant figures.

2. GENERAL PROPERTIES

2.1 Definitions

$$\Xi(x) = \int_0^x e^{-\xi^2} \int_0^\xi e^{\zeta^2} \int_0^\zeta e^{-t^2} dt d\zeta d\xi, \tag{2.1}$$

$$\Xi(x) = \frac{\sqrt{\pi}}{2} \int_0^x e^{-\xi^2} \int_0^\xi e^{\zeta^2} \mathit{erf}(\zeta) d\zeta d\xi, \tag{2.2}$$

$$\Xi'(x) = e^{-x^2} \int_0^x e^{\zeta^2} \int_0^\zeta e^{-t^2} dt d\zeta, \tag{2.3}$$

$$\Xi'(x) = \frac{\sqrt{\pi}}{2} e^{-x^2} \int_0^x e^{\zeta^2} \mathit{erf}(\zeta) d\zeta. \tag{2.4}$$

2.2 Differential Equation

$$\Xi'' + 2x\Xi' = \frac{\sqrt{\pi}}{2} \mathit{erf}(x), \qquad \Xi(0) = \Xi'(0) = 0. \tag{2.5}$$

2.3 Integral Representation

$$\Xi(x) = -\frac{1}{2\sqrt{\pi}} \int_0^\infty e^{-p^2/4} \frac{\sin(px)}{p} [\ln(p) + \frac{\gamma}{2}] dp. \tag{2.6}$$

2.4 Symmetry Relations

$$\Xi(-x) = -\Xi(x), \tag{2.7}$$

$$\Xi'(-x) = \Xi'(x). \tag{2.8}$$

2.5 Series Expansions

$$\Xi(x) = \frac{e^{-x^2}}{4} \sum_{j=1}^{\infty} \frac{2^j d_j}{(2j+1)!!} x^{2j+1}, \qquad |x| < \infty. \tag{2.9}$$

Here $d_j = \gamma + \psi(j+1) = \sum_{k=1}^{j} k^{-1}$.

$$\Xi'(x) = \frac{e^{-x^2}}{4} \sum_{j=1}^{\infty} \frac{2^j}{j(2j-1)!!} x^{2j}, \qquad |x| < \infty, \tag{2.10}$$

$$\Xi(x) = \frac{1}{2} \sum_{j=1}^{\infty} \frac{(-1)^{j+1} c_j}{(2j+1)j!} x^{2j+1}, \qquad |x| < \infty, \tag{2.11}$$

$$\Xi'(x) = \frac{1}{2} \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j!} c_j x^{2j}, \qquad |x| < \infty. \tag{2.12}$$

In (2.11) and (2.12), $c_j = \ln(2) + \frac{\gamma}{2} + \frac{1}{2}\psi(j+1/2) = \sum_{i=1}^{j} (2i-1)^{-1}$.

2.6 Asymptotic expansions

$$\Xi(x) \sim \frac{\sqrt{\pi}}{4} \left[\ln(x) + \frac{\gamma}{2} - \frac{1}{2} \sum_{j=1}^{\infty} \frac{(2j-1)!!}{j 2^j x^{2j}} \right], \qquad x \to \infty \tag{2.13}$$

$$\Xi'(x) \sim \frac{\sqrt{\pi}}{4} \sum_{j=0}^{\infty} \frac{(2j-1)!!^{\dagger}}{2^j x^{2j+1}}, \qquad x \to \infty. \tag{2.14}$$

2.7 Expression as a series of incomplete gamma functions

$$\Xi(x) = \frac{\sqrt{\pi}}{8} \sum_{j=1}^{\infty} \frac{1}{j\Gamma(j+1/2)} \gamma(j+1/2, x^2). \tag{2.15}$$

† for negative argument the double factorial is defined to be identically equal to one.

2.8 Relation to Dawson's Integral

$$\Xi'(x) = \frac{\sqrt{\pi}}{2}\, \mathit{erf}(x)F(x) - e^{-x^2}\int_0^x F(t)dt. \tag{2.16}$$

2.9 Maximum of $\Xi'(x)$

$$\Xi'(1.379005630....) = 0.3048918974..., \tag{2.17}$$

$$\Xi\ (1.379005630....) = 0.2257293172.... \tag{2.18}$$

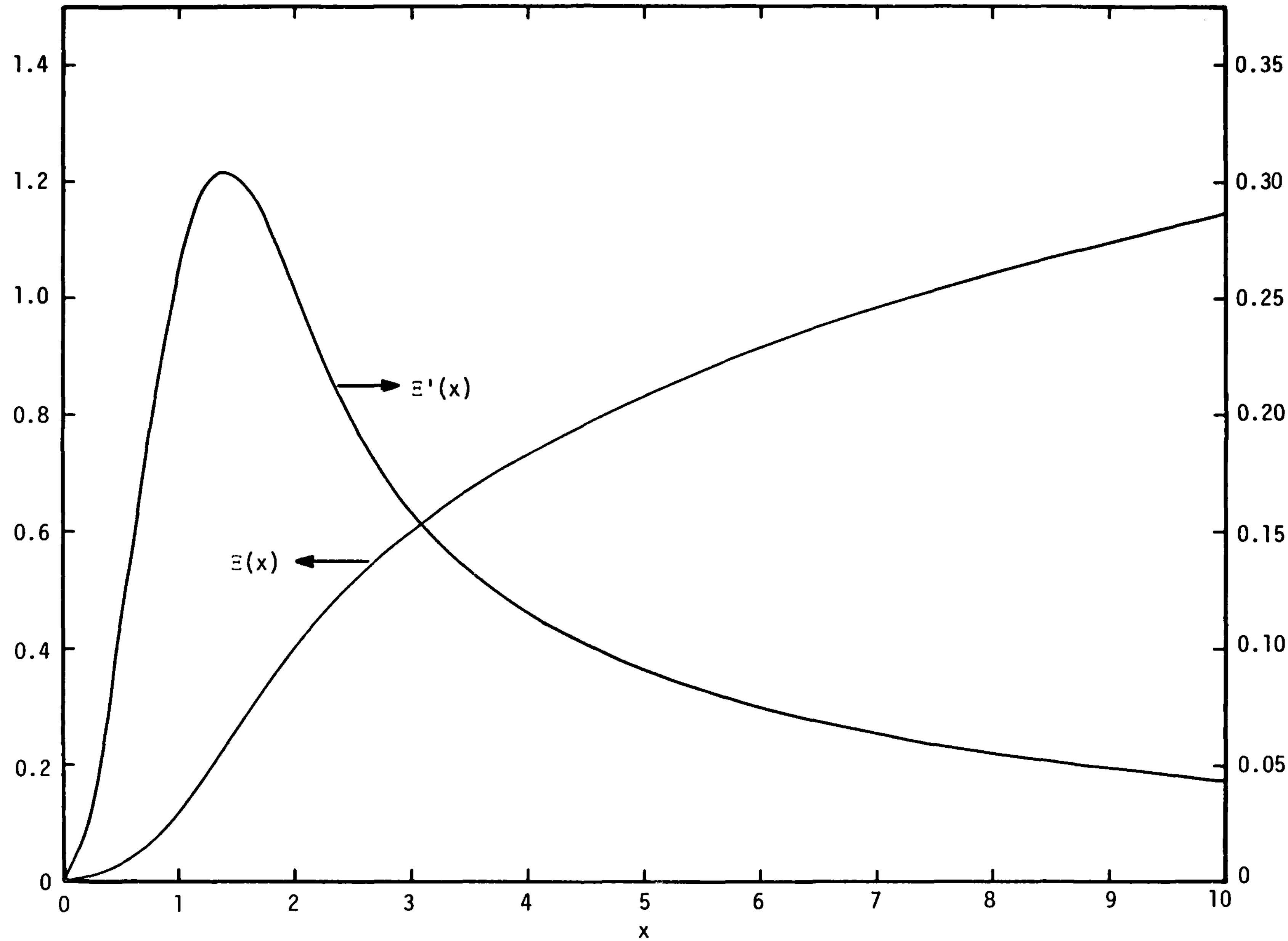

Figure 1. Graphs of $\Xi(x)$ and $\Xi'(x)$ on a linear x-scale.

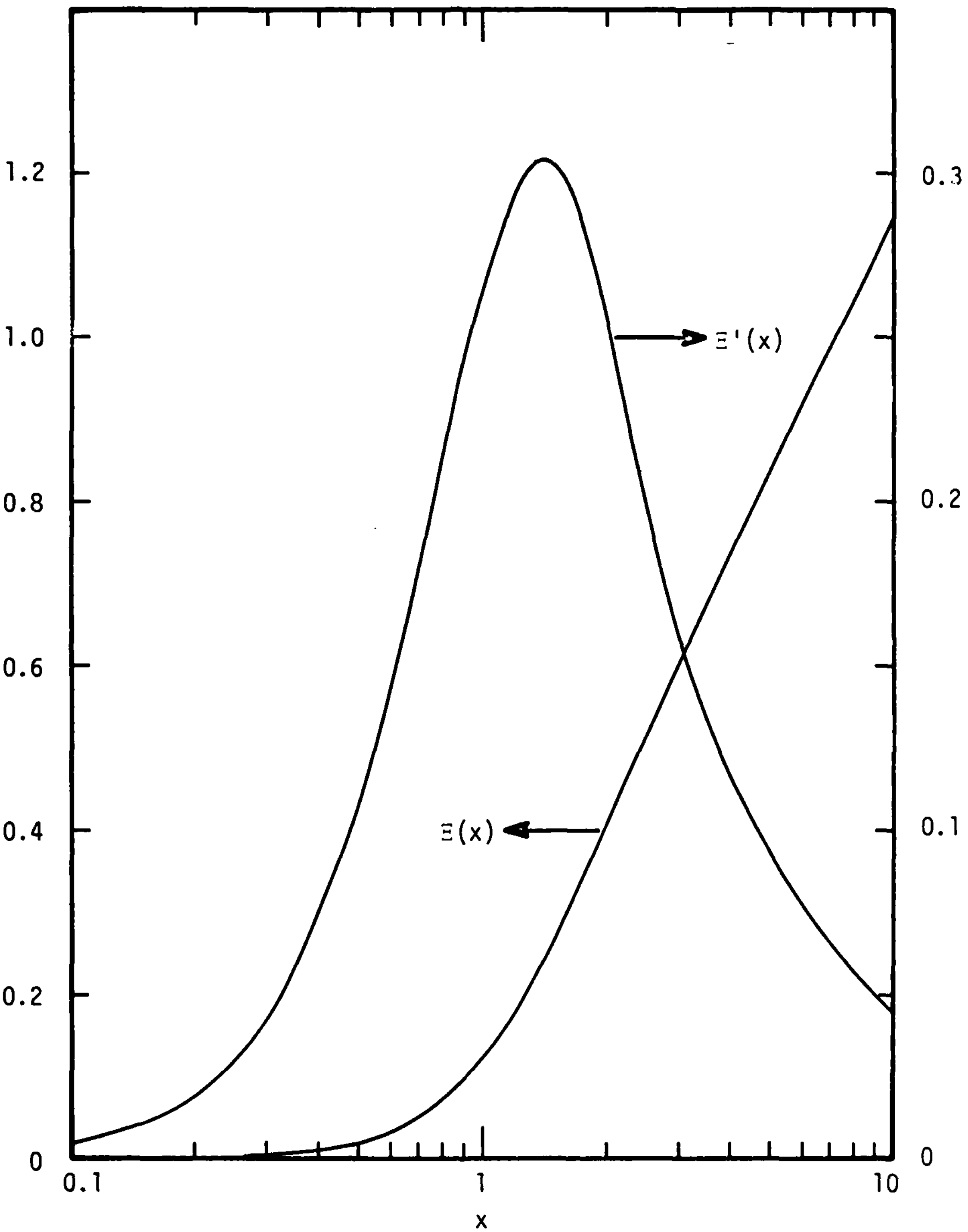

Figure 2. Graphs of $\Xi(x)$ and $\Xi'(x)$ on a logarithmic x-scale.

3. INTEGRALS

3.1 Combination of Ξ and Ξ' with Powers

1. $$\int \Xi(ax)dx = x\Xi(ax) + \frac{1}{2a}\Xi'(ax) - \frac{\sqrt{\pi}}{4} x\,\mathrm{erf}(ax) - \frac{1}{4a} e^{-a^2x^2},$$

2. $$\int x\Xi(ax)dx = \frac{(2a^2x^2 - 1)}{4a^2}\Xi(ax) + \frac{x}{4a}\Xi'(ax) - \frac{\sqrt{\pi}}{32a^2}(2a^2x^2-1)\mathrm{erf}(ax) - \frac{x}{16a} e^{-a^2x^2},$$

3. $$\int x^n\Xi(ax)dx = p_1(a,x)\Xi(ax) + p_2(a,x)\Xi'(ax) + p_3(a,x)\mathrm{erf}(ax) + p_4(a,x)e^{-a^2x^2},$$

In 3.1 3 for n a positive even integer, viz. $n = 2k$ with $k = 0,1,2,\ldots$:

$$p_1 = \frac{x^{2k+1}}{2k+1}, \quad p_2 = \frac{k!}{2(2k+1)a^{2k+1}} \sum_{j=0}^{k} \frac{1}{j!}(ax)^{2j}$$

$$p_3 = -\frac{\sqrt{\pi}\,k!}{4(2k+1)a^{2k}} \sum_{j=0}^{k} \frac{a^{2j}}{(2j+1)j!} x^{2j+1},$$

$$p_4 = -\frac{k!}{4(2k+1)a^{2k+1}} \sum_{j=0}^{k} \frac{1}{j!}(ax)^{2j}(c_{k+1} - c_j),$$

where c_j is defined in (2.12) for $j \geq 1$ and $c_0 = 0$. In 3.1 3 for n a positive odd integer, viz. $n = 2k + 1$ with $k = 0,1,2,3,\ldots$:

$$p_1 = \frac{1}{2(k+1)}\left[x^{2k+2} - \frac{(2k+1)!!}{2^{k+1}a^{2k+2}}\right],$$

$$p_2 = \frac{(2k+1)!!}{2^{k+2}a^{2k+2}(k+1)}\sum_{j=0}^{k}\frac{2^j}{(2j+1)!!}(ax)^{2j+1},$$

$$p_3 = -\frac{\sqrt{\pi}\,(2k+1)!!}{2^{k+4}a^{2k+2}(k+1)}\left[\sum_{j=0}^{k}\frac{2^j}{(j+1)(2j+1)!!}(ax)^{2j+2} - \frac{1}{2}d_{k+1}\right],$$

$$p_4 = -\frac{(2k+1)!!}{2^{k+4}a^{2k+2}(k+1)}\sum_{j=0}^{k}\frac{2^j}{(2j+1)!!}(ax)^{2j+1}(d_{k+1} - d_j),$$

where d_j is defined in (2.9) for $j \geq 1$ and here $d_0 = 0$.

4. $$\int x\Xi'(ax)dx = -\frac{1}{2a^2}\Xi'(ax) + \frac{\sqrt{\pi}}{4a}\,x\,\mathrm{erf}(ax) + \frac{1}{4a^2}e^{-a^2x^2},$$

5. $$\int x^n\Xi'(ax)dx = \frac{x^n}{a}\Xi(ax) - \frac{n}{a}\int x^{n-1}\Xi(ax)dx,$$

for n integer and $n \geq 1$.

6. $$\int_0^x \Xi'(at)\frac{dt}{t} = \frac{1}{4}\sum_{j=1}^{\infty}\frac{(-1)^{j+1}c_j}{jj!}(ax)^{2j}, \qquad |ax| < \infty,$$

where c_j is defined in (2.12).

7. $$\int_0^\infty \Xi'(ax)\frac{dx}{x} = \frac{\pi^2}{16},$$

8. $$\int_0^x \Xi(at)\frac{dt}{t} = \frac{1}{2}\sum_{j=1}^{\infty}\frac{(-1)^{j+1}c_j}{(2j+1)^2 j!}(ax)^{2j+1}, \qquad |ax| < \infty,$$

where c_j is defined in (2.12),

$$9.\quad \int \Xi(ax)\,\frac{dx}{x^2} = -\frac{1}{x}\,\Xi(ax) + a\int \Xi'(ax)\,\frac{dx}{x}\,,$$

$$10.\quad \int \Xi(ax)\,\frac{dx}{x^3} = -\left[a^2 + \frac{1}{2x^2}\right]\Xi(ax) - \frac{a}{2x}\,\Xi'(ax)$$

$$+\frac{\sqrt{\pi}}{4}\,a^2\,\mathit{erfei}(ax),$$

where the function $\mathit{erfei}(x)$ is discussed in Appendix A.

$$11.\quad \int \Xi'(ax)\,\frac{dx}{x^2} = -\frac{1}{x}\,\Xi'(ax) - 2a\Xi(ax) + \frac{\sqrt{\pi}}{2}\,a\,\mathit{erfei}(ax),$$

$$12.\quad \int \Xi'(ax)\,\frac{dx}{x^n} = -\frac{1}{n-1}\left[\frac{1}{x^{n-1}}\,\Xi'(ax) + \frac{a\sqrt{\pi}}{2(n-2)x^{n-2}}\,\mathit{erf}(ax)\right.$$

$$\left.+\frac{a^{n-1}}{2(n-2)}\,\Gamma\!\left(\frac{3-n}{2}\,,\,a^2x^2\right) + 2a^2\int \Xi'(ax)\,\frac{dx}{x^{n-2}}\right],$$

for $n \geq 3$. In 3.1 12, for n an even integer, viz. $n = 2k+2$ with $k = 1,2,3...$

$$\Gamma\!\left(\frac{3-n}{2}\,,\,a^2x^2\right) = \frac{(-1)^k}{\Gamma\!\left(\frac{2k+1}{2}\right)}\left[e^{-a^2x^2}\sum_{i=1}^{k}\frac{(-1)^i\,\Gamma\!\left(\frac{2i-1}{2}\right)}{(ax)^{2i-1}} + \pi\,\mathit{erfc}(ax)\right],$$

while for n, an odd integer, viz. $n = 2k+1$ with $k = 1,2,3,...$

$$\Gamma\!\left(\frac{3-n}{2}\,,\,a^2x^2\right) = \frac{(-1)^{k-1}}{(k-1)!}\left[e^{-a^2x^2}\sum_{i=1}^{k-1}\frac{(-1)^i\,\Gamma(i)}{(ax)^{2i}} + E_1(a^2x^2)\right]^{\dagger}.$$

$$13.\quad \int \Xi(ax)\,\frac{dx}{x^n} = -\frac{1}{(n-1)}\left[\frac{\Xi(ax)}{x^{n-1}} - a\int \Xi'(ax)\,\frac{dx}{x^{n-1}}\right],\quad n \geq 2,$$

---

† for $k = 1$ the summation term is identically zero.

3.2 Combinations of Ξ and Ξ' with Exponentials and Powers

$$1. \quad \int_0^x e^{-t^2}\Xi'(t)dt = \frac{1}{2}\sum_{j=1}^{\infty} \frac{a_j}{(2j+1)} x^{2j+1}, \qquad |x| < \infty.$$

Here

$$a_j = \frac{(-1)^{j+1}}{j!} \sum_{i=1}^{j} \binom{j}{i} c_i ,$$

where c_i is defined in (2.12).

$$2. \quad \int_0^{\infty} e^{-x^2}\Xi'(ax)dx = \frac{1}{8}\sqrt{\frac{\pi}{a^2+1}}\, \ln(a^2+1),$$

$$3. \quad \int xe^{-x^2}\Xi'(x)dx = -\frac{e^{-x^2}}{4}\Xi'(x) + \frac{\pi}{32}\,\mathrm{erf}^2(x),$$

$$4. \quad \int x^2e^{-x^2}\Xi'(x)dx = -\frac{x}{4}e^{-x^2}\Xi'(x) - \frac{\sqrt{\pi}}{16}e^{-x^2}\mathrm{erf}(x) + \frac{\sqrt{2\pi}}{32}\mathrm{erf}(\sqrt{2}x)$$
$$+ \frac{1}{4}\int e^{-x^2}\Xi'(x)dx,$$

$$5. \quad \int x^3e^{-x^2}\Xi'(x)dx = -\frac{1}{8}(2x^2+1)e^{-x^2}\Xi'(x) + \frac{\pi}{32}\mathrm{erf}^2(x)$$
$$- \frac{\sqrt{\pi}}{16}xe^{-x^2}\mathrm{erf}(x) - \frac{1}{32}e^{-2x^2},$$

$$6. \quad \int x^ne^{-x^2}\Xi'(x)dx = -\frac{x^{n-1}}{4}e^{-x^2}\Xi'(x) + \frac{\sqrt{\pi}}{8}\int x^{n-1}e^{-x^2}\mathrm{erf}(x)dx$$
$$+ \frac{(n-1)}{4}\int x^{n-2}e^{-x^2}\Xi'(x)dx.$$

For the evaluation of the second term on the right side of equation 3.2 6 the following reduction formulae are useful:

$$\int x^{n-1}e^{-x^2}\mathit{erf}(x)dx = -\frac{x^{n-2}}{2}e^{-x^2}\mathit{erf}(x) + \frac{1}{\sqrt{\pi}}\int x^{n-2}e^{-2x^2}dx$$

$$+\frac{(n-2)}{2}\int x^{n-3}e^{-x^2}\mathit{erf}(x)dx,$$

$$\int x^{n-1}e^{-2x^2}dx = -\frac{x^{n-2}}{4}e^{-2x^2} + \frac{(n-2)}{4}\int x^{n-3}e^{-2x^2}dx,$$

7. $\int_0^x e^{-t^2}\Xi(t)dt = \sum_{j=1}^{\infty} b_j x^{2j+2},$

where

$$b_j = \frac{(-1)^{j+1}}{4(j+1)!}\sum_{i=1}^{j}\binom{j}{i}\frac{c_i}{2i+1},$$

and c_i is defined in (2.12).

8. $\int_0^\infty e^{-t^2}\Xi(t)dt = \frac{G}{8} - \frac{\pi}{32}\ell n(2),$

where G is Catalan's constant.

9. $\int xe^{-x^2}\Xi(x)dx = -\frac{e^{-x^2}}{2}\Xi(x) + \frac{1}{2}\int e^{-x^2}\Xi'(x)dx,$

10. $\int x^n e^{-x^2}\Xi(x)dx = -\frac{x^{n-1}}{2}e^{-x^2}\Xi(x) + \frac{1}{2}\int x^{n-1}e^{-x^2}\Xi'(x)dx$

$$+\frac{(n-1)}{2}\int x^{n-2}e^{-x^2}\Xi(x)dx.$$

For the evaluation of the second term on the right side of 3.2 10 see 3.2 6.

11. $\int_0^x e^{-t^2}\Xi'(t)\,\frac{dt}{t} = \frac{1}{4}\sum_{j=1}^{\infty}\frac{a_j}{j}x^{2j}, \qquad |x| < \infty,$

where a_j is defined in 3.2 1.

12. $\int_0^\infty e^{-t^2}\Xi'(at)\,\frac{dt}{t} = \frac{\pi^2}{16} - \frac{1}{4}\,\mathrm{arcot}(a)[\pi - \mathrm{arcot}(a)], \quad -\infty < a < \infty,$

13. $$\int_0^x e^{-t^2}\Xi'(t)\,\frac{dt}{t^2} = -\frac{e^{-x^2}}{x}\,\Xi'(x) - 4\int_0^x e^{-t^2}\Xi'(t)dt + \frac{\pi}{8}\,\frac{\mathrm{erf}^2(x)}{x}$$

$$+ \frac{\pi}{8}\int_0^x \mathrm{erf}^2(t)\,\frac{dt}{t^2},$$

14. $\int_0^\infty e^{-t^2}\Xi'(t)\,\frac{dt}{t^2} = \frac{\sqrt{\pi}}{2}\,\ln(1+\sqrt{2}) - \frac{\sqrt{2\pi}}{4}\,\ln(2),$

15. $$\int_x^\infty e^{-t^2}\Xi'(t)\frac{dt}{t^n} = \frac{e^{-x^2}}{(n-1)x^{n-1}}\,\Xi'(x) - \frac{4}{(n-1)}\int_x^\infty e^{-t^2}\Xi'(t)\,\frac{dt}{t^{n-2}}$$

$$+ \frac{\sqrt{\pi}}{2(n-1)}\int_x^\infty e^{-t^2}\mathrm{erf}(t)\,\frac{dt}{t^{n-1}},$$

for $n \geq 2$.

16. $\int_0^x e^{-t^2}\Xi(t)\,\frac{dt}{t} = \sum_{j=1}^{\infty}\frac{2(j+1)}{2j+1}\,b_j x^{2j+1}, \qquad |x| < \infty,$

where b_j is defined in 3.2 7.

17. $\int_0^\infty e^{-t^2}\Xi(t)\,\frac{dt}{t} = 0.047128\ 94918,$

$$18. \quad \int e^{-x^2}\Xi(x)\,\frac{dx}{x^n} = -\frac{e^{-x^2}}{(n-1)x^{n-1}}\,\Xi(x) - \frac{2}{(n-1)}\int e^{-x^2}\Xi(x)\,\frac{dx}{x^{n-2}}$$

$$+ \frac{1}{(n-1)}\int e^{-x^2}\,\Xi'(x)\,\frac{dx}{x^{n-1}}\,,$$

for $n \geq 2$.

3.3 Combinations of Ξ and Ξ' with the Error function and Powers

$$1. \quad \int \mathrm{erf}(x)\Xi'(x)dx = \mathrm{erf}(x)\Xi(x) - \frac{2}{\sqrt{\pi}}\int e^{-x^2}\Xi(x)dx,$$

$$2. \quad \int \mathrm{erf}(x)\Xi(x)dx = \left[x\,\mathrm{erf}(x) + \frac{e^{-x^2}}{\sqrt{\pi}}\right]\Xi(x) + \frac{1}{2}\,\mathrm{erf}(x)\Xi'(x)$$

$$- \frac{2}{\sqrt{\pi}}\int e^{-t^2}\,\Xi'(t)dt$$

$$- \frac{\sqrt{\pi}}{4}\left[x\,\mathrm{erf}^2(x) + \frac{2}{\sqrt{\pi}}\,e^{-x^2}\mathrm{erf}(x) - \sqrt{\frac{2}{\pi}}\,\mathrm{erf}(\sqrt{2}x)\right],$$

$$3. \quad \int x\,\mathrm{erf}(x)\Xi'(x)dx = -\frac{1}{2}\,\mathrm{erf}(x)\Xi'(x) + \frac{1}{\sqrt{\pi}}\int e^{-t^2}\,\Xi'(t)dt$$

$$+ \frac{\sqrt{\pi}}{4}\,x\,\mathrm{erf}^2(x) + \frac{1}{2}\,e^{-x^2}\mathrm{erf}(x) - \frac{\sqrt{2}}{4}\,\mathrm{erf}(\sqrt{2}x),$$

$$4. \quad \int x\,\mathrm{erf}(x)\Xi(x)dx = \left[\frac{(2x^2-1)}{4}\,\mathrm{erf}(x) + \frac{1}{2\sqrt{\pi}}\,xe^{-x^2}\right]\Xi(x)$$

$$+ \frac{1}{4}\left[x\,\mathrm{erf}(x) + \frac{e^{-x^2}}{\sqrt{\pi}}\right]\Xi'(x) - \frac{\sqrt{\pi}}{16}\,x^2\mathrm{erf}^2(x)$$

$$- \frac{1}{8}\,xe^{-x^2}\mathrm{erf}(x) - \frac{1}{16\sqrt{\pi}}\,e^{-2x^2},$$

5. $\int x^n erf(x)\Xi'(x)dx = x^n erf(x)\Xi(x) - \frac{2}{\sqrt{\pi}}\int x^n e^{-x^2}\Xi(x)dx$

$$- n\int x^{n-1} erf(x)\Xi(x)dx.$$

For evaluation of the second term on the right side of 3.3 5 see 3.2 10.

3.4 Combinations of Ξ and Ξ' with Logarithms and Powers

1. $\int_0^x \ln(t)\Xi'(t)dt = \ln(x)\Xi(x) - \int_0^x \frac{\Xi(t)}{t}\,dt,$

2. $\int_0^x \ln(t)\Xi(t)dt = \left[x\Xi(x) + \frac{1}{2}\Xi'(x) - \frac{\sqrt{\pi}}{4}x\,erf(x) - \frac{e^{-x^2}}{4} + \frac{1}{4}\right]\cdot$

$$\left[\ln(x) - 1\right] + \frac{\sqrt{\pi}}{4}x\,erf(x) + \frac{1}{4}\left[e^{-x^2} - 1\right] - \frac{1}{8}E_1(x^2)$$

$$- \frac{1}{4}\ln(x) - \frac{\gamma}{8} - \frac{1}{2}\int_0^x \Xi'(t)\frac{dt}{t},$$

3. $\int_0^x t\ln(t)\Xi'(t)dt = -\left[\frac{1}{2}\Xi'(x) - \frac{\sqrt{\pi}}{4}x\,erf(x) - \frac{1}{4}e^{-x^2} + \frac{1}{4}\right]\ln(x)$

$$+ \frac{1}{2}\int_0^x \Xi'(t)\frac{dt}{t} - \frac{\sqrt{\pi}}{4}x\,erf(x) - \frac{1}{4}(e^{-x^2} - 1)$$

$$+ \frac{1}{8}[E_1(x^2) + 2\ln(x) + \gamma],$$

4. $\int_0^x t\ln(t)\Xi(t)dt = \left[\frac{(2x^2-1)}{4}\Xi(x) + \frac{x}{4}\Xi'(x) - \frac{\sqrt{\pi}}{32}(2x^2 - 1)erf(x)\right.$

$$\left. - \frac{x}{16}e^{-x^2}\right]\cdot\left[\ln(x) - \frac{1}{2}\right] - \frac{1}{4}\Xi(x) + \frac{1}{4}\int_0^x \Xi(t)\frac{dt}{t}$$

$$+ \frac{\sqrt{\pi}}{32}\left[x^2 erf(x) + \frac{1}{\sqrt{\pi}}xe^{-x^2} + \frac{1}{2}erf(x) - erfei(x)\right].$$

3.5 Miscellaneous Integrals

1. $$\int_0^x e^{a^2t^2} \mathrm{erf}(at)dt = \frac{2}{a\sqrt{\pi}} e^{a^2x^2} \Xi'(ax),$$

2. $$\int_0^x e^{t^2} \mathrm{erf}^2(t)dt = \frac{2}{\sqrt{\pi}} e^{x^2} \mathrm{erf}(x)\Xi'(x) - \frac{4}{\pi} \Xi(x),$$

3. $$\int_0^x e^{t^2} \mathrm{erf}^3(t)dt = \frac{2}{\sqrt{\pi}} e^{x^2} \mathrm{erf}^2(x)\Xi'(x) - \frac{8}{\pi} \mathrm{erf}(x)\Xi(x)$$
$$+ \frac{16}{\pi\sqrt{\pi}} \int_0^x e^{-t^2} \Xi(t)dt,$$

4. $$\int_0^x e^{t^2} \mathrm{erfc}^2(t)\mathrm{erf}(t)dt = \frac{2}{\sqrt{\pi}} \mathrm{erfc}^2(x)e^{x^2} \Xi'(x) + \frac{8}{\pi} \mathrm{erfc}(x)\Xi(x)$$
$$+ \frac{16}{\pi\sqrt{\pi}} \int_0^x e^{-t^2} \Xi(t)dt,$$

5. $$\int_0^x e^{t^2} \mathrm{erfc}(\sqrt{2}t)\mathrm{erf}(t)dt = \frac{2}{\sqrt{\pi}} \mathrm{erfc}(\sqrt{2}x)e^{x^2} \Xi'(x)$$
$$+ \frac{4\sqrt{2}}{\pi} \int_0^x e^{-t^2} \Xi'(t)dt.$$

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APPENDIX A: THE FUNCTION ERFEI(x)

In integrals 3.1 10, 3.1 11 and 3.4 4, the function defined by equation (A.1) arises. In this Appendix, some useful properties of this function are given; the function is plotted in figure A.1 and tabulated in table A.1

A.1 Definition

$$\mathcal{erfei}(x) = \int_0^x \frac{\mathcal{erf}(t)}{t}\,dt.$$

A.2 Integral Representation

$$\mathcal{erfei}(x) = -\frac{2}{\sqrt{\pi}}\,x\int_0^1 e^{-x^2t^2}\,\ell n(t)\,dt, \qquad |x| < \infty.$$

A.3 Symmetry Relation

$$\mathcal{erfei}(-x) = -\,\mathcal{erfei}(x).$$

A.4 Series Expansion

$$\mathcal{erfei}(x) = \frac{2}{\sqrt{\pi}}\sum_{j=0}^{\infty}\frac{(-1)^j}{(2j+1)^2 j!}\,x^{2j+1}, \qquad |x| < \infty.$$

A.5 Asymptotic Expansions

$$\mathcal{erfei}(x) \sim \ell n(2x) + \frac{\gamma}{2} + \frac{e^{-x^2}}{2\sqrt{\pi}\,x^3}\left[1 - \frac{2}{x^2} + \frac{23}{4x^4} - \frac{22}{x^6} + \frac{1689}{16x^8} - \frac{4881}{8x^{10}} + \dots\right], \qquad x \to \infty.$$

A.6 Indefinite Integrals

1. $$\int \mathit{erfei}(x)dx = x\,\mathit{erfei}(x) - x\,\mathit{erf}(x) - \frac{1}{\sqrt{\pi}} e^{-x^2},$$

2. $$\int x^n \mathit{erfei}(x)dx = \frac{1}{n+1} x^{n+1} \mathit{erfei}(x) - \frac{1}{(n+1)^2} x^{n+1} \mathit{erf}(x)$$

$$+ \frac{1}{(n+1)^2\sqrt{\pi}} \gamma(1 + \frac{n}{2}, x^2).$$

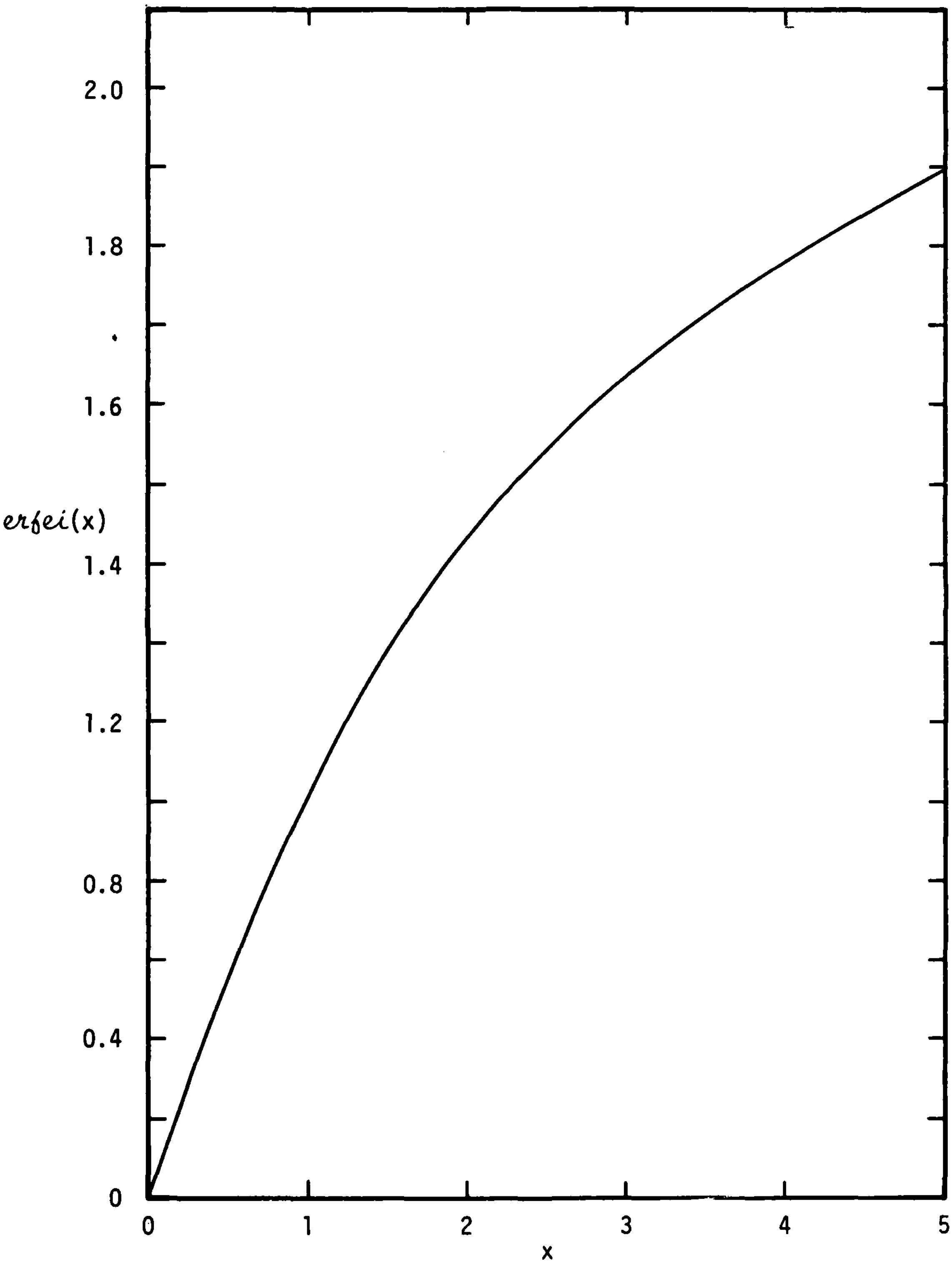

Figure A.1. The function $erfei(x)$

TABLE A.1[†]

x	$erfei(x)$	x	$erfei(x)$
0.00	0.00000 00000	2.00	1.67535 04327
0.10	0.11271 27665	2.10	1.72395 62837
0.20	0.22468 00025	2.20	1.77036 53206
0.30	0.33518 26238	2.30	1.81475 13483
0.40	0.44355 25900	2.40	1.85727 26708
0.50	0.54919 39999	2.50	1.89807 27340
0.60	0.65159 93946	2.60	1.93728 10996
0.70	0.75036 04607	2.70	1.97501 45953
0.80	0.84517 28573	2.80	2.01137 85246
0.90	0.93583 54106	2.90	2.04646 78598
1.00	1.02224 43601	3.00	2.08036 83701
1.10	1.10438 36667	3.10	2.11315 76561
1.20	1.18231 25702	3.20	2.14490 60827
1.30	1.25615 16257	3.30	2.17567 76063
1.40	1.32606 83591	3.40	2.20553 05035
1.50	1.39226 35013	3.50	2.23451 80088
1.60	1.45495 85267	3.60	2.26268 88709
1.70	1.51438 49639	3.70	2.29008 78382
1.80	1.57077 57076	3.80	2.31675 60822
1.90	1.62435 83548	3.90	2.34273 15672
		4.00	2.36804 93746

[†]Values of $erfei(x)$ for $x > 4$ (correct to ten significant figures) may be obtained by using the first two terms of A.5.

APPENDIX B: FORTRAN FUNCTION ROUTINE AND TABULATED VALUES OF $\Xi(x)$ AND $\Xi'(x)$

In Table B.1, the listing of a function subprogram is given for the numerical evaluation of $\Xi(x)$ and $\Xi'(x)$. The functions $\Xi(x)$ and $\Xi'(x)$ are accessed from the calling program by,

```
Y = XI(X,EPSI,IERR)   ,   Y = XIP(X,EPSI,IERR),
```

respectively. In these calling statements

X ≡ the argument of either $\Xi(x)$ or $\Xi'(x)$,

EPSI ≡ the assigned tolerance which is dependent of the number of significant figures desired for $\Xi(x)$ or $\Xi'(x)$,

IERR ≡ an integer variable returned by the function subprogram. (IERR = 0 if the tolerance EPSI is met; IERR = 1 otherwise.)

The subprogram accepts only zero or positive values of x and returns a zero value if $x < 0$. If the evaluation of $\Xi(x)$ or $\Xi'(x)$ is required for $x < 0$, the calling statement should reflect the appropriate symmetry relation (either (2.7) or (2.8)).

For $x < 5.0$ the routine evaluates $\Xi(x)$ and $\Xi'(x)$ using the power series expansions (2.9) and (2.11) in the DO loops commencing with cards 20 and 29, respectively. The power series in (2.9) and (2.10) are summed until they have converged to the number of significant figures dictated by the assigned value of the tolerance EPSI; once convergence occurs control is transferred out of the DO loops to statements 3 or 5, respectively. The DO loops commencing

with cards 20 and 29 are initially set (by card 11) so that at most 100 terms in either power series will be evaluated. If convergence occurs before the DO loops are satisfied, a reliable result has been obtained and IERR = 0 is returned to the calling program. If the DO loops are satisfied, the returned value of $\Xi(x)$ or $\Xi'(x)$ may not be reliable to the specified tolerance (EPSI) and IERR = 1 is returned to the calling program.

For $x \geq 5.0$, the asymptotic expansions (2.13) and (2.14) are used for the evaluation of Ξ and Ξ'. The sums in (2.13) and (2.14) are evaluated in the DO loops commencing with cards 38 and 46, respectivley. Control is transferred out of these DO loops when the last term added to these sums is less than the desired exit tolerance EPSI; again a returned value of IERR = 1 indicates this condition has not been met after 100 terms in the series have been summed.

Computed values of Ξ and Ξ' are given in Table B.2; these values were evaluated with EPSI = 10^{-12} and are correct to ten significant figures (the last digit is rounded off). The CPU time required to produce the entire table was 0.842 seconds on a CDC 6500. The storage required for XI is 171 words. The program was written for a CDC machine; for computers which operate with less presision, XI may easily be modified for double precision if a high degree of accuracy is needed.

```
      FUNCTION XI(X,EPSI,IERR)
      DATA SRPI,GAM0/1.772453850905516,0.57721566490153286/
      XI=0$IF=1
      IF(X.LE.0.) RETURN
      GO TO 1
      ENTRY XIP
      XI=0.$IF=2
      IF(X.LE.0.) RETURN
1     X2=X*X
      FAC=2.*X2
      M=100
      IERR=0
      SUM=0.
      SUMT=0.
      TERM=1.
      IF(X.GE.5.) GO TO 110
      IF(IF.EQ.2) GO TO 100
      TERM=X
      ALPHA=1.
      DO 2 I=1,M
      TERM=TERM*FAC/FLOAT(2*I+1)
      SUM=SUM+TERM*ALPHA
      IF(ABS((SUM-SUMT)/SUM).LT.EPSI) GO TO 3
      ALPHA=ALPHA+1./FLOAT(I+1)
2     SUMT=SUM
      IERR=1
3     XI=0.25*EXP(-X2)*SUM
      RETURN
100   DO 4 I=1,M
      TERM=TERM*FAC/FLOAT(2*I-1)
      SUM=SUM+TERM/FLOAT(I)
      IF(ABS((SUM-SUMT)/SUM).LT.EPSI) GO TO 5
4     SUMT=SUM
      IERR=1
5     XI=0.25*EXP(-X2)*SUM
      RETURN
110   IF(IF.EQ.2) GO TO 120
      DO 6 I=1,M
      TERM=TERM*FLOAT(2*I-1)/FAC
      TERMA=TERM/FLOAT(I)
      IF(TERMA.LT.EPSI) GO TO 7
6     SUM=SUM+TERMA
      IERR=1
7     XI=SRPI*(ALOG(X2)+GAM0-SUM)/8.
      RETURN
120   DO 8 I=1,M
      TERM=TERM*FLOAT(2*I-1)/FAC
      IF(TERM.LT.EPSI) GO TO 9
8     SUM=SUM+TERM
      IERR=1
9     XI=SRPI*(1.+SUM)/(4.*X)
      RETURN
      END
```

Table B.1. FORTRAN function routine for the numerical evaluation of $\Xi(x)$ and $\Xi'(x)$

TABLE B.2

x	Ξ(x)	Ξ'(x)	x	Ξ(x)	Ξ'(x)
0.00	0.00000 00000	0.00000 00000	5.00	0.83647 55948	(-1)0.90513 96674
0.10	(-3)0.16600 18215	(-2)0.49667 94096	5.10	0.84543 37558	(-1)0.88662 31905
0.20	(-2)0.13122 31678	(-1)0.19474 75580	5.20	0.85421 05888	(-1)0.86886 59127
0.30	(-2)0.43419 16955	(-1)0.42390 90215	5.30	0.86281 34482	(-1)0.85182 10068
0.40	(-1)0.10012 91790	(-1)0.71967 91837	5.40	0.87124 92399	(-1)0.83544 55111
0.50	(-1)0.18885 34957	0.10603 37513	5.50	0.87952 44578	(-1)0.81969 99290
0.60	(-1)0.31290 22308	0.14221 74031	5.60	0.88764 52166	(-1)0.80454 78777
0.70	(-1)0.47321 19062	0.17818 00344	5.70	0.89561 72816	(-1)0.78995 57812
0.80	(-1)0.66848 42292	0.21182 20008	5.80	0.90344 60950	(-1)0.77589 25981
0.90	(-1)0.89550 98227	0.24144 25483	5.90	0.91113 68005	(-1)0.76232 95830
1.00	0.11496 21681	0.26583 80743	6.00	0.91869 42648	(-1)0.74924 00732
1.10	0.14252 14171	0.28433 51804	6.10	0.92612 30976	(-1)0.73659 93004
1.20	0.17162 64540	0.29676 42616	6.20	0.93342 76696	(-1)0.72438 42224
1.30	0.20168 03441	0.30338 65749	6.30	0.94061 21293	(-1)0.71257 33729
1.40	0.23212 96272	0.30479 17529	6.40	0.94768 04176	(-1)0.70114 67264
1.50	0.26249 14660	0.30178 34527	6.50	0.95463 62820	(-1)0.69008 55781
1.60	0.29236 94322	0.29526 87699	6.60	0.96148 32891	(-1)0.67937 24349
1.70	0.32145 89291	0.28616 31134	6.70	0.96822 48360	(-1)0.66899 09175
1.80	0.34954 41840	0.27531 74919	6.80	0.97486 41616	(-1)0.65892 56716
1.90	0.37648 92054	0.26347 05669	6.90	0.98140 43556	(-1)0.64916 22887
2.00	0.40222 51381	0.25122 40720	7.00	0.98784 83683	(-1)0.63968 72325
2.10	0.42673 61718	0.23903 76697	7.10	0.99419 90188	(-1)0.63048 77738
2.20	0.45004 56933	0.22723 80552	7.20	1.0004 59002	(-1)0.62155 19304
2.30	0.47220 38365	0.21603 69560	7.30	1.0066 30898	(-1)0.61286 84121
2.40	0.49327 70769	0.20555 32997	7.40	1.0122 17176	(-1)0.60442 65712
2.50	0.51334 00923	0.19583 58849	7.50	1.0187 20202	(-1)0.59621 63571
2.60	0.53246 98095	0.18688 40873	7.60	1.0246 42244	(-1)0.58822 82742
2.70	0.55074 13614	0.17866 52362	7.70	1.0304 85478	(-1)0.58045 33441
2.80	0.56822 55924	0.17112 81812	7.80	1.0362 51993	(-1)0.57288 30702
2.90	0.58498 77346	0.16421 31835	7.90	1.0419 43795	(-1)0.56550 94057
3.00	0.60108 69077	0.15785 86265	8.00	1.0475 62811	(-1)0.55832 47240
3.10	0.61657 61587	0.15200 51934	8.10	1.0531 10895	(-1)0.55132 17913
3.20	0.63150 28204	0.14659 81709	8.20	1.0585 89830	(-1)0.54449 37413
3.30	0.64590 90301	0.14158 84599	8.30	1.0640 01331	(-1)0.53783 40521
3.40	0.65983 23067	0.13693 27628	8.40	1.0693 47051	(-1)0.53133 65247
3.50	0.67330 61180	0.13259 32920	8.50	1.0746 28582	(-1)0.52499 52632
3.60	0.68636 04075	0.12853 72415	8.60	1.0798 47458	(-1)0.51880 46560
3.70	0.69902 20615	0.12473 61723	8.70	1.0850 05160	(-1)0.51275 93591
3.80	0.71131 53151	0.12116 54032	8.80	1.0901 03113	(-1)0.50685 42801
3.90	0.72326 20998	0.11780 34521	8.90	1.0951 42696	(-1)0.50108 45635
4.00	0.73488 23379	0.11463 15474	9.00	1.1001 25240	(-1)0.49544 55768
4.10	0.74619 41927	0.11163 32117	9.10	1.1050 52029	(-1)0.48993 28979
4.20	0.75721 42797	0.10879 39140	9.20	1.1099 24305	(-1)0.48454 23034
4.30	0.76795 78461	0.10610 07801	9.30	1.1147 43268	(-1)0.47926 97571
4.40	0.77843 89246	0.10354 23[illegible]34	9.40	1.1195 10081	(-1)0.47411 14000
4.50	0.78867 04646	0.10110 83963	9.50	1.1242 25865	(-1)0.46906 35404
4.60	0.79866 44457	(-1)0.98789 72500	9.60	1.1288 91708	(-1)0.46412 26451
4.70	0.80843 19760	(-1)0.96578 07181	9.70	1.1335 08663	(-1)0.45928 53306
4.80	0.81798 33776	(-1)0.94465 96875	9.80	1.1380 77749	(-1)0.45454 83557
4.90	0.82732 82618	(-1)0.92446 64968	9.90	1.1425 99954	(-1)0.44990 86135
			10.00	1.1470 76236	(-1)0.44536 31249

END
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